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Livello bibliografico	Monografia
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Nota di bibliografia	Includes bibliographical references and indexes.
Nota di contenuto	1. Elementary wave mechanics; 2. Density matrices; 3. Density-functional theory; 4. The chemical potential; 5. Chemical potential derivatives; 6. Thomas-Fermi and related models; 7. The Kohn-Sham method: Basic principles; 8. The Kohn-Sham method: Elaboration; 9. Extensions; 10. Aspects of atoms and molecules; 11. Miscellany; Appendices: A. Functionals. B. Convex functions and functionals. C. Second quantization for fermions. D. The Wigner Distribution Function and the \hbar semiclassical expansion. E. The uniform electron gas. F. Tables of values of electronegativities and hardnesses. G. The review literature of density-functional theory
Sommario/riassunto	This text is a rigorous, unified account of the fundamental principles of the density-functional theory of the electronic structure of matter and its applications to atoms and molecules. Containing a detailed discussion of the chemical potential and its derivatives, it provides an understanding of the concepts of electronegativity, hardness and softness, and chemical reactivity. Both the Hohenberg-Kohn-Sham and the Levy-Lieb derivations of the basic theorems are presented, and extensive references to the literature are included. Two introductory chapters and several appendices provide all the background material necessary beyond a knowledge of elementary quantum theory. The volume is intended for physicists, chemists, and advanced students in chemistry.